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UPGRADED LINE-OF-SIGHT GEOMETRY PACKAGE AND BAND MODEL PARAMETERS FOR MODTRAN

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The MODTRAN atmospheric transmittance and radiance code was upgraded with new band model parameters calculated using the HITRAN-92 line atlas. The (1/d) band model parameters for O_3 were adjusted to give better agreement with the corresponding line-by-line FASCOD3 calculations for long paths in the 20-50 km altitude region. More accurate line-of-sight (LOS) geometry routines were incorporated for greater consistency between the geometry parameters. Furthermore, MODTRAN can now handle very short slant paths down to 0.001 km.

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1. INTRODUCTION

MODTRAN[1,2] is a new atmospheric radiance-transmittance code based on LOWTRAN with increased spectral resolution. LOWTRAN 7,[3,4] the latest LOWTRAN code, calculates atmospheric transmittance and radiance for arbitrary lines-of-sight (LOS's) at 20 cm^{-1} resolution in steps of 5 cm^{-1} from 0 to 50,000 cm^{-1}. The code uses a single-parameter band model and altitude scaling functions for molecular line absorption. It also includes aerosol and molecular continuum-type absorption plus single and multiple scattering effects. MODTRAN has all these capabilities plus a spectral resolution of 2 cm^{-1} (full-width at half-maximum, FWHM). It uses a temperature- and pressure-dependent two-parameter band model for molecular absorption and transmission calculations while the other parts of the calculation remain unchanged from those in LOWTRAN. In fact, the regular LOWTRAN calculations remain as a user-specified MODTRAN option.

The geometry routines in MODTRAN and LOWTRAN allow the user several different input options for unambiguously specifying the LOS. The routines compute the unspecified path parameters and output a "complete set" of LOS parameters. However, for some particular geometries, the output parameters are often different from the input ones. This is noticeable for slant paths specified by range and zenith angle, especially those paths which are near-horizontal, and many input sets where the LOS is only a few kilometers or less. These problems were eliminated by upgrading the geometry package. In implementing the upgrades, changes to the routines and the number of new routines were kept to a minimum to facilitate validation.

A second effort was to upgrade the MODTRAN band model parameters using the latest HITRAN line atlas. Additionally, in the 20-50 km altitude region and for paths longer than 100 km, MODTRAN ozone transmittances were found to be higher than the corresponding line-by-line FASCOD3[5] calculations. In light of this, the MODTRAN line density parameters for ozone were adjusted for a much better fit with FASCOD3.

Modifications to the MODTRAN LOS geometry are described in Section 2, and calculation of the new band model parameters are described in Section 3. For brevity, we use MODTRAN to denote the old geometry package in both LOWTRAN 7 and MODTRAN, and MODTRAN2 to denote the new geometry package. MODTRAN2 will also refer to the latest band model parameters.

2. THE LOS GEOMETRY PACKAGE

This section discusses modifications to the geometry routines. First, we describe how the various LOS paths are characterized in MODTRAN and what the different input schemes for specifying the LOS's are. Second, we describe the problem areas and our approach for eliminating them. Illustrative examples are given.

2.1 LOS Specification

The input parameters for characterizing a general LOS path are listed in Table 1. It is to be noted that HMIN is also the tangent altitude for long paths (like limb views from a high altitude platform) that go down to a minimum altitude (the tangent point) and then increase in altitude. The three generic path types recognized by MODTRAN are listed in Table 2. The type is selected by assigning the appropriate value to the input variable ITYPE. The ITYPE = 3 path is a special case of ITYPE = 2 where H2 is space, that is, the outer boundary of the highest atmospheric layer (typically 100 km).

Table 1. The LOS Parameters.

H1	sensor or observer altitude
H2	source altitude
ANGLE	zenith angle at H1
BETA	earth-center angle
RANGE	distance along the LOS between H1 and H2
HMIN	minimum altitude of the LOS

Table 2. Path Types Reorganized in MODTRAN.

ITYPE	PATH DESCRIPTION
1	horizontal homogeneous path with constant temperature, pressure and concentrations
2	vertical or slant path between H1 and H2
3	vertical or slant path to space from H1

For slant paths, ITYPE = 2, one of four parameter sets are used to uniquely specify a path. They are H1 and two additional parameters. Table 3 lists the four possibilities each identified by a CASE label: 2A, 2B, 2C, or 2D. These CASE designations are internal to MODTRAN and are not seen by the user. Some input schemes are converted into other equivalent schemes for subsequent calculations. Since the most convenient parameter set for tracing a ray through the atmosphere and calculating absorber amounts is CASE 2A, all paths are eventually converted to this case. CASE 2B is converted to 2A by determining H2. CASE 2C is converted to 2D by determining BETA, and finally both 2C and 2D are converted to 2A by determining ANGLE. So accuracy problems in one case can manifest themselves in other cases.

Table 3. Parameter Sets for ITYPE = 2 Paths.

CASE LABEL	SPECIFIED PARAMETERS
2A	H1, H2, ANGLE
2B	H1, ANGLE, RANGE
2C	H1, H2, RANGE
2D	H1, H2, BETA

2.2 Geometry Issues

The mismatch between the input and output LOS parameters are confined to some slant paths specified by ITYPE = 2 and 3. The reasons for it have been traced to these areas:

1. Simple numerical precision problems;
2. Calculation of H2 without refraction effects for CASE 2B;
3. Convergence problems in determining ANGLE for CASES 2C and 2D; and
4. Short slant paths.

Since ITYPE = 3 is a special case of ITYPE = 2 and utilizes the same routines, the upgrades to the ITYPE = 2 LOS's automatically carry over the to ITYPE = 3.

Our approach was to:

1. Improve the numerical accuracy and stability of some algorithms;
2. Fix remaining problems with refraction and convergence for slant paths with ranges exceeding 2 km; and
3. Accommodate short slant paths with ranges less than 2 km.

The first and most obvious changes made improved the numerical accuracy of the computed parameters. These changes fixed many but not all the problems. We then examined and fixed all ITYPE = 2 slant paths, case by case. Finally, we tackled the case of short slant paths with ranges less than 2 km. For these short ranges, we ignore atmospheric refraction.

2.3 Improving Numerical Accuracy

Some FORTRAN statements in MODTRAN could be replaced by identical equivalents that are numerically more stable. As an example, the expression

$$R_1^2 + R_2^2 - 2R_1R_2 \cos\beta \tag{1}$$

where $R_i = R_e + H_i$, $i = 1, 2$ and R_e = earth radius, is more appropriately coded as

$$(H_1 - H_2)^2 + 4R_1R_2 \sin^2\frac{\beta}{2} \quad . \tag{2}$$

In the first expression, the third term nearly equals the sum of the first two terms for small values of β. The inclusion of R_e^2 in all terms means that, for small β, a large number is subtracted from another number of comparable magnitude. This leads to significant loss of accuracy. The second expression, on the other hand, is more accurate because some R_e's have been eliminated.

Another method for improving numerical accuracy for small β is to use a Taylor series expansion:

$$(H_1 - H_2)^2 - R_1R_2 \left(- \frac{\beta^6}{135} + \frac{\beta^4}{12} - \beta^2\right) \quad . \tag{3}$$

It is worthwhile to note that in summing up a series of terms in a computer, it is more accurate to start with the smaller terms. That is why the sextuple term is first in the expansion.

In addition, a number of FORTRAN variables, perhaps a few more than really necessary, were changed from single to double precision.

Improving the numerical accuracy was sufficient to get agreement among input and output parameters for CASE 2A (H1, H2, ANGLE) and many input sets for CASE 2C (H1, H2, RANGE). However, these improvements did not produce agreement among the parameters for all CASE 2C inputs. The main problem areas were CASE 2D (H1, H2, BETA) and CASE 2B (H1, H2, RANGE).

Table 4 compares the MODTRAN and MODTRAN2 output ranges for various CASE 2C inputs. For small input ranges, MODTRAN output ranges differ greatly from the input values. For input ranges of 2.0, 6.0, and 20.0 km, MODTRAN did not yield any output values. The reason is that, after these CASE 2C inputs were converted to CASE 2D, the computation of ANGLE did not converge.

Table 4. Examples for CASE 2C with H1 = 5 and H2 = 5 km.

	RANGE (km)	
INPUT	MODTRAN	MODTRAN2
2.01	—	2.00
4.7	5.31	4.72
6.0	—	6.01
8.0	7.51	8.01
9.0	7.51	9.01
10.0	9.20	10.02
20.0	—	20.01
50.0	50.51	50.02
100.0	100.52	100.01
200.0	199.96	200.01
300.0	300.13	300.01

2.4 Slant Paths - CASEs 2B & 2D

The only remaining problems with slant paths, which did not fall into the category of short slant paths, were with CASE 2B and CASE 2D inputs. Consistency for the 2B cases was obtained by determining H2 by a refractive calculation when converting to 2A. A modified iterative procedure for determining BETA gives better convergence for the 2D cases.

CASE 2B (H1, ANGLE, RANGE)

The LOS path for this case was converted to CASE 2A by computing H2, but without refraction. Once H2 is calculated, CASE 2A proceeds by including atmospheric refraction effects. A set of routines was written to include refraction in the initial H2 calculation. As a result, the input and output parameters are now in agreement as shown in Table 5. Since refraction bends the rays towards the earth, the H2 values calculated with refraction (MODTRAN2) are consistently less than those calculated via straight line geometry (MODTRAN).

Table 5. Examples for CASE 2B with H1 = 5 km and ANGLE = 92°.

	RANGE (km)		H2 (km)	
INPUT	MODTRAN	MODTRAN2	MODTRAN	MODTRAN2
10	10	10	4.66	4.66
50	49	50	3.45	3.43
100	96	100	2.29	2.20
150	136	150	1.53	1.30
200	162	200	1.16	0.74
250	358	250	1.18	0.52
300	385	300	1.59	0.64
350	427	350	2.39	1.11

The value of H2 with refraction is calculated by summing the differential elements of range, ds, along the LOS from H1 to H2. The most convenient variable of integration is the radial distance, r, of a point on the ray from the center of the earth. Thus H2 is the altitude at which the integrated path length equals the input RANGE. This method of determining H2 is non-iterative and quick. For details, the reader is referred to Kneizys et al.[3]

CASE 2D (H1, H2, BETA)

For this case, MODTRAN computes ANGLE iteratively. Initially, an educated guess of ANGLE based on straight line geometry is made, and the corresponding BETA is computed by including refraction. If this computed BETA does not agree with the input, a new guess of ANGLE is made, and the process is repeated until convergence. If the iteration does not converge, the calculations are skipped. A new iterative algorithm based on a Newton-Raphson scheme was found to consistently give better convergence. In this scheme, ANGLE is incremented by an amount based on its derivative with respect to BETA. The examples shown in Table 4 for which MODTRAN did not yield any output ranges were caused by convergence problems with CASE 2D (to which all CASE 2C schemes are converted). MODTRAN2, on the other hand, yields accurate output ranges for these input schemes.

2.5 Short Slant Paths

Short slant paths are defined as paths whose lengths lie between a meter and two kilometers. These had to be treated differently from the general slant paths, because even in double precision the refractive calculations were numerically unstable.

Since refraction is insignificant at these ranges, we ignore it. All short slant paths are converted into CASE 2A. A DATA statement in the routine DRIVER governs the value of the switch (currently 2 km) for short slant paths. The MODTRAN2 pathlength-dependent quantities match at 2 km. The user should be aware of this switch if he is performing detailed studies around this range.

3. MODTRAN BAND MODEL PARAMETERS

MODTRAN uses band model parameters, calculated directly from the HITRAN line atlas, for these twelve molecular species: H_2O, CO_2, O_3, N_2O, CO, CH_4, O_2, NO, SO_2, NO_2, NH_3, and HNO_3. These parameters were upgraded using the latest version, HITRAN'92.[6] In addition, it was noted by the Phillips Laboratory that the MODTRAN O_3 transmittances for long paths in the 20-50 km altitude regime differed significantly from the more exact line-by-line FASCOD3 calculations. This, most acute in the ν_3 9.6 μm region and shown in Figure 1, was traced to the band model line density parameters (1/d). It was found that a slightly variant version of the previous (1/d) formalism gave better overall agreement with the FASCODE results. The O_3 transmittance computed using the new line density parameters is also displayed in Figure 1.

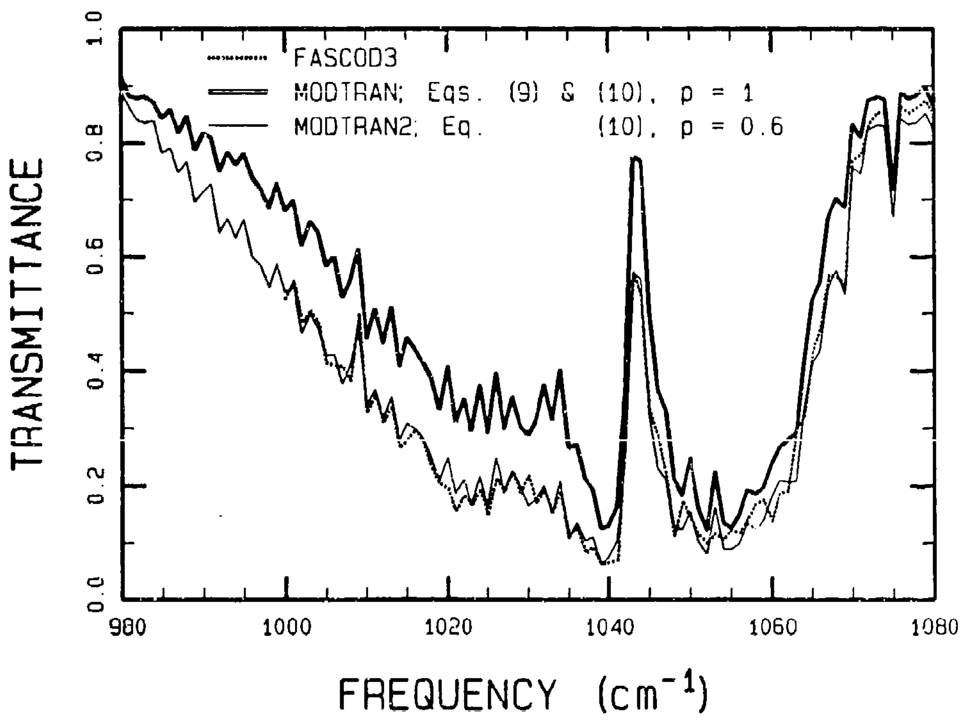

Figure 1. Comparison of MODTRAN (Heavy Solid Line) and FASCOD3 (Dotted Line) Ozone Transmittances for a Homogeneous Path of RANGE = 500 km at H1 = 30 km. Also Shown is the MODTRAN2 Calculation (Light Solid Line). The Calculations were Performed at 1 cm^{-1} Resolution.

This section describes the upgrades to the current band model parameters including the new (1/d) parameters for ozone. A brief formalism describing the band model is presented first.

3.1 Formulation of the Band Model Parameters

The MODTRAN band model parameters are derived and explained in the original MODTRAN reports,[1,2] so only an overview is presented here. Band models assume that the line strengths and locations are statistical, and their accuracy increases as both the bin size and number of lines increase. Model parameters are determined by requiring agreement in the strong- and weak-line limits of the transmittance expressions.

In MODTRAN, the molecular transmittance, τ, from lines originating within a spectral bin, $\Delta\nu$, is given by

$$\tau = \left(\frac{2}{\Delta\nu} \int_0^{\Delta\nu/2} e^{-S\,u\,b(\nu)}\, d\nu \right)^n \quad , \tag{4}$$

where $b(\nu)$ is the Voigt line shape function, u is the absorber amount, and S and n are defined in terms of the absorption coefficient (S/d) and line density (1/d) band model parameters:

$$S = \frac{(S/d)}{(1/d)} \tag{5}$$

$$n = (1/d)\,\Delta\nu \quad . \tag{6}$$

Roughly speaking, n is the average number of lines, and S is the average line strength in the bin.

The standard expressions, due to Goody,[7] for the two parameters are given by

$$(S/d) = \frac{1}{\Delta\nu} \sum_{i=1}^{N} S_i \tag{7}$$

$$(1/d) \approx \frac{1}{\Delta\nu} (\sum_{i=1}^{N} \sqrt{S_i})^2 / \sum_{i=1}^{N} S_i \quad . \tag{8}$$

Here N is the number of lines whose centers are contained in the bin and S_i is the integrated strength of line i. The line density formula assumes that all N lines have the same half-width. Equations (7) and (8) are derived from the strong- and weak-line limits of the Ladenburg-Reiche function.[7] However, Equation (8) may not be completely appropriate for MODTRAN because the Ladenburg-Reiche function gives the total absorption due to N lines and not just the contribution within a finite spectral bin as does Equation (4).[1,2] Therefore, a modified formulation for (1/d) is used in MODTRAN.

If the strong- and weak-line limits of Plass' expression[8] is equated to Equation (4) to model the transmission due to lines whose centers are randomly distributed in any given spectral interval, the expression for (1/d) becomes:

$$(1/d) \approx \frac{1}{\Delta\nu} (\sum_{i=1}^{N} S_i)^2 \; / \; \sum_{i=1}^{N} S_i^2 \tag{9}$$

(S/d) has the same form as Equation (7). In this formulation, the contributions from the "tails" of lines centered outside a bin are treated separately. The latter formula for (1/d) has a smaller value than the former because the weaker lines are weighted less in Equation (9) than in Equation (8).

3.2 New Band Model Parameters

The original MODTRAN band model parameters are based on the HITRAN'86[9] line atlas. They were recalculated using HITRAN'92.[6] As before, the MODTRAN band model parameters are computed at 1 cm^{-1} intervals and for 5 reference temperatures: 200, 225, 250, 275, and 300 K. Except for ozone, the band model parameters for the remaining molecules are calculated using Equations (7) and (9). The ozone parameters are described in the next subsection. A new tape file representing the latest band model parameters replaces the old one.

3.3 The Ozone Band Model Parameters

The new formulation of (1/d), Equation (9), was judged to be more appropriate than Equation (8) for all molecules in MODTRAN. However, it now appears that a value of (1/d) that lies somewhere in between Equations (8) and (9) is best for ozone. In fact, the FASCODE ozone transmittances at various altitudes and for a wide range of optical depths are "sandwiched" by MODTRAN transmittance curves calculated with Equations (8) and (9). A typical example is shown in Figure 2.

To develop an empirical form for (1/d), it is convenient to recast both Equations (8) and (9) as:

$$(1/d) \approx \frac{1}{\Delta\nu} \left(\sum S_i^p\right)^2 / \sum S_i^{2p} \tag{10}$$

where p varies between 0.5 (Equation (8)) and 1.0 (Equation (9)). By trial and error, we

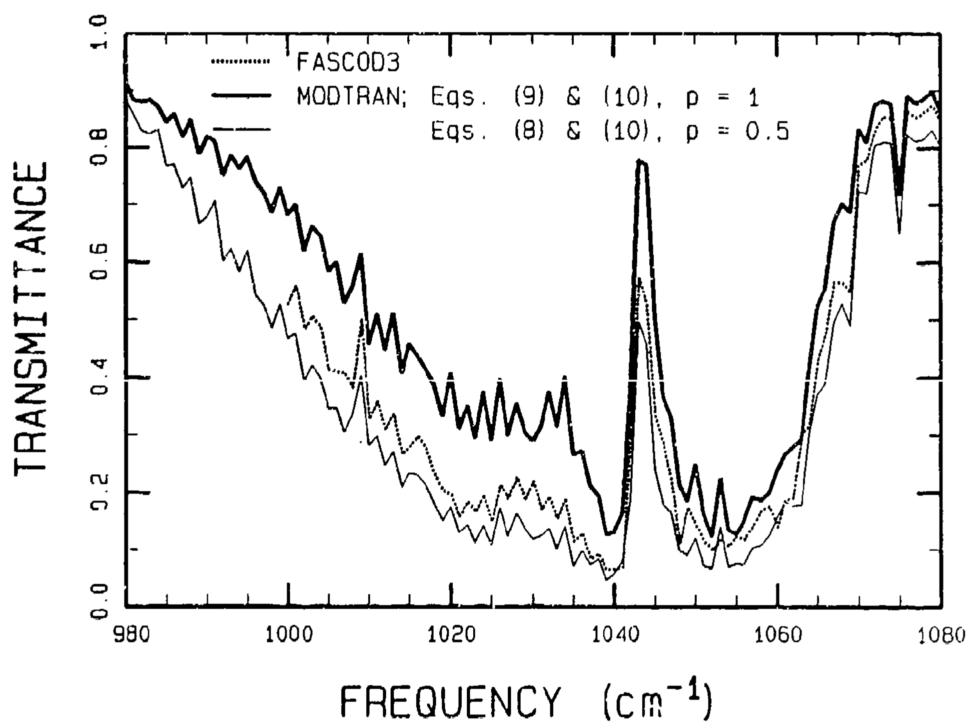

Figure 2. Comparison of FASCOD3 Ozone Transmittance with those Calculated Using Equations (8) and (9) for the Path Described in Figure 1.

found that $p = 0.6$ yielded the best overall agreement between MODTRAN and FASCOD3 for a variety of ozone transmittances at various altitudes and ranges. Therefore, the new ozone (1/d) parameters were calculated by setting $p = 0.6$ in Equation (10). The (S/d) formulation of Equation (7) remained unchanged. Figures 1 and 3-6 show several transmittance calculations at different altitudes and path lengths. The calculations of Figure 1 were performed at a resolution of 1 cm^{-1}; all others were performed at a resolution of 2 cm^{-1}.

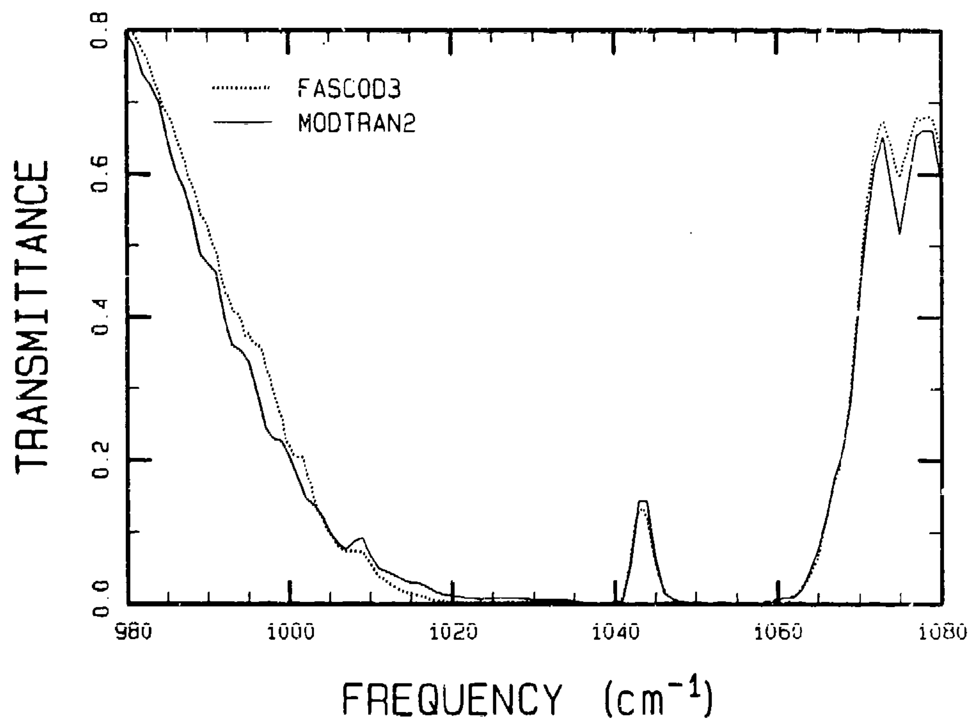

Figure 3. Comparison of MODTRAN2 and FASCOD3 Transmittance Calculations at 20 km for a Horizontal Path of 500 km in the 9.6 μm $O_3(\nu_3)$ Region.

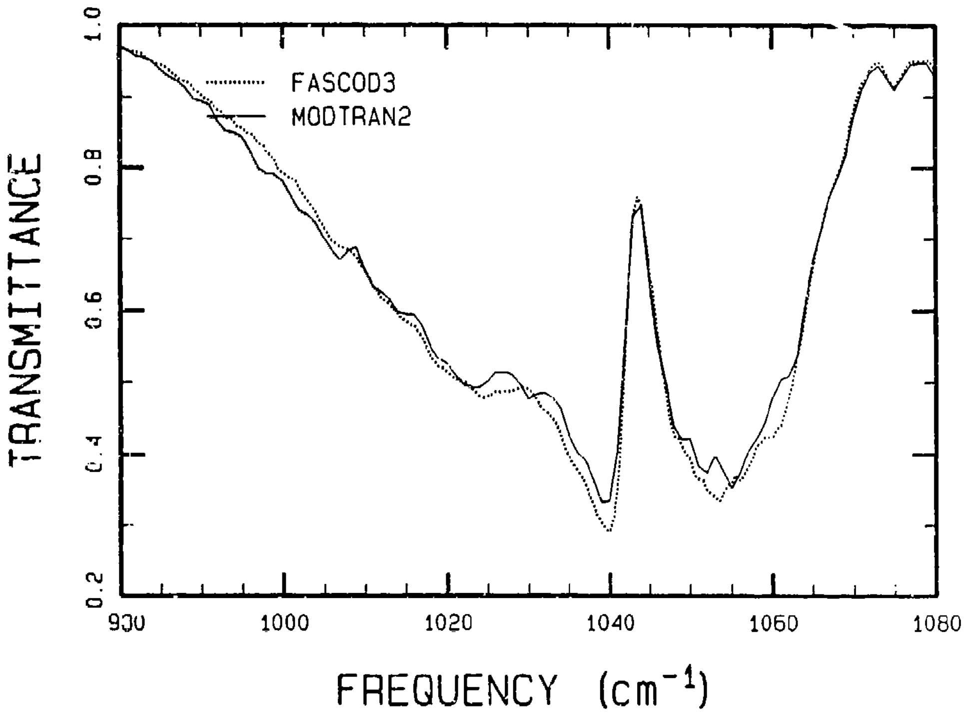

Figure 4. Comparison of MODTRAN2 and FASCOD3 Transmittance Calculations at 30 km for a Horizontal Path of 100 km in the 9.6 μm $O_3(\nu_3)$ Region.

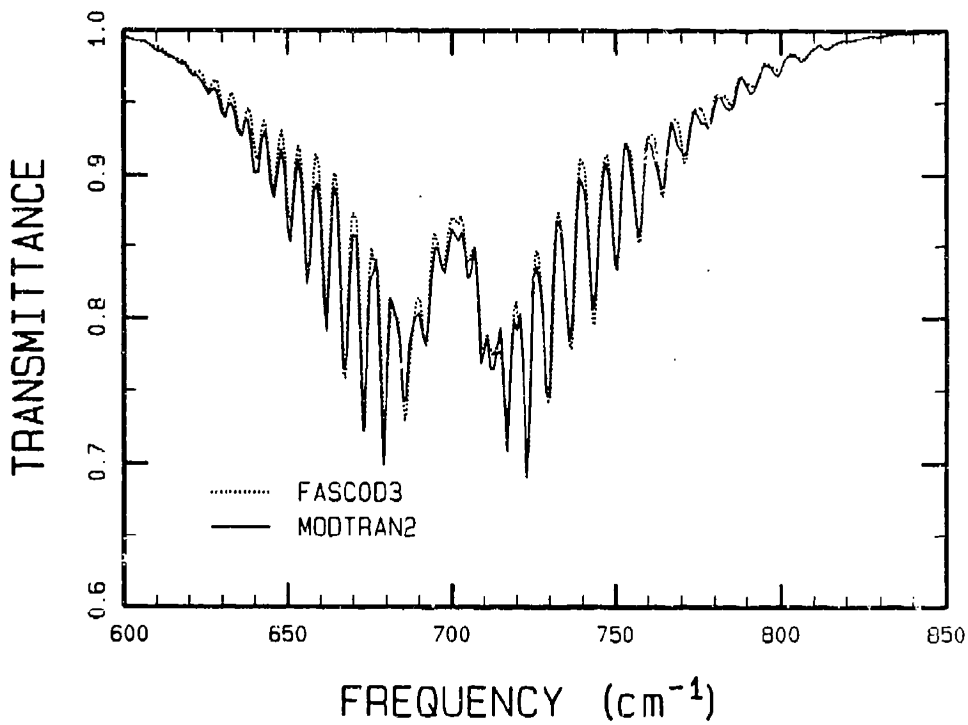

Figure 5. Comparison of MODTRAN2 and FASCOD3 Transmittance Calculations at 30 km for a Horizontal Path of 500 km in the 14 μm $O_3(\nu_2)$ Region.

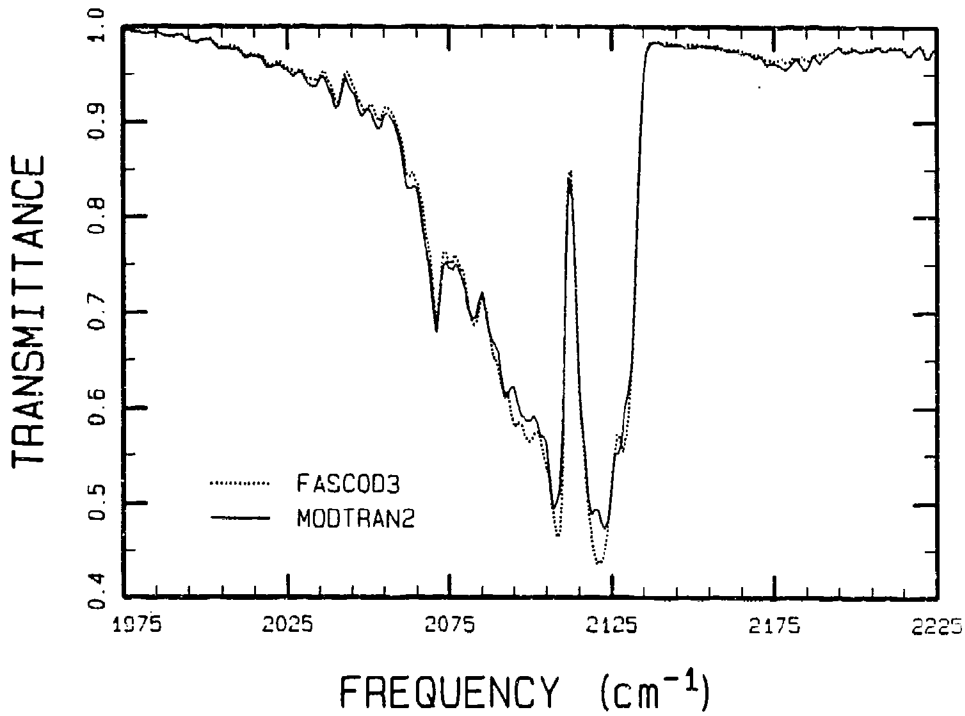

Figure 6. Comparison of MODTRAN2 and FASCOD3 Transmittance Calculations at 30 km for a Horizontal Path of 500 km in the 4.8 μm $O_3(\nu_1 + \nu_3)$ Region.

4. SUMMARY

The geometry package in MODTRAN was modified so that the actual line-of-sight (LOS) parameters used for the transmittance/radiance calculations always closely match the user's requested or input values. The geometry routines incurred round-off problems on 32-bit machines due to subtraction of large numbers. The new routines replace numerically unstable algebraic expressions by more stable identities and occasionally resort to double precision arithmetic. Two other upgrades were the calculation of H2 with refraction effects for the case specified by (H1, ANGLE, RANGE) and a new iterative algorithm for the case specified by (H1, H2, BETA). Furthermore, new modules and modifications can now handle short slant paths, those whose lengths are less than 2 km, by ignoring refraction.

A second effort was to upgrade the MODTRAN band model parameters using the latest HITRAN'92 line atlas. Additionally, in the 20-50 km altitude region and for paths longer than 100 km, MODTRAN ozone transmittances are higher than the corresponding line-by-line FASCOD3 calculations. In light of this, the line density parameters for ozone were adjusted somewhat upward for a much better fit with FASCOD3.

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